

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentanediol $\geq 99\%$, for synthesis

article number: **CN17**
Version: **GHS 4.0 en**
Replaces version of: 2024-03-02
Version: (GHS 3)

date of compilation: 2020-10-22
Revision: 2024-03-15

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Identification of the substance	2-Methyl-2,4-pentanediol $\geq 99\%$, for synthesis
Article number	CN17
CAS number	107-41-5
Alternative name(s)	Hexyleneglucol

1.2 Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household). Food, drink and animal feeding-stuffs.

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

Telephone: +49 (0) 721 - 56 06 0
Telefax: +49 (0) 721 - 56 06 149
e-mail: sicherheit@carlroth.de
Website: www.carlroth.de

Competent person responsible for the safety data sheet: Department Health, Safety and Environment

e-mail (competent person): sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 Westmead, NSW	131126	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
2.6	Flammable liquid	4	Flam. Liq. 4	H227
3.2	Skin corrosion/irritation	2	Skin Irrit. 2	H315
3.3	Serious eye damage/eye irritation	2	Eye Irrit. 2	H319

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentandiol $\geq 99\%$, for synthesis

article number: **CN17**

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.7	Reproductive toxicity	2	Repr. 2	H361d

For full text of abbreviations: see SECTION 16

The most important adverse physicochemical, human health and environmental effects

The product is combustible and can be ignited by potential ignition sources.

2.2 Label elements

Labelling

Signal word

Warning

Pictograms

GHS07, GHS08



Hazard statements

H227	Combustible liquid
H315	Causes skin irritation
H319	Causes serious eye irritation
H361d	Suspected of damaging the unborn child

Precautionary statements

Precautionary statements - prevention

P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking
P280	Wear protective gloves

Precautionary statements - response

P302+P352	IF ON SKIN: Wash with plenty of soap and water
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P308+P313	IF exposed or concerned: Get medical advice/attention
P337+P313	If eye irritation persists: Get medical advice/attention
P370+P378	In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction

Precautionary statements - disposal

P501	Dispose of contents/container to industrial combustion plant
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For professional users only

2.3 Other hazards

This material is combustible, but will not ignite readily.

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentanediol $\geq 99\%$, for synthesis

article number: CN17

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	2-Methyl-2,4-pentanediol
Molecular formula	$C_6H_{14}O_2$
Molar mass	118.2 g/mol
CAS No	107-41-5

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

Following ingestion

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

4.2 Most important symptoms and effects, both acute and delayed

Vomiting, Irritation, Headache, Cough, Vertigo, Spasms, Dyspnoea, Unconsciousness

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!
water spray, alcohol resistant foam, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentanediol $\geq 99\%$, for synthesis

article number: CN17

5.2 Special hazards arising from the substance or mixture

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours may form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Use personal protective equipment as required. Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains.

Advice on how to clean up a spill

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation. Avoid exposure.

Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentanediol ≥99 %, for synthesis

article number: CN17

Take precautionary measures against static discharge.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ventilation requirements

Use local and general ventilation.

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Country	Name of agent	CAS No	Identifier	TWA [ppm]	TWA [mg/m ³]	STEL [ppm]	STEL [mg/m ³]	Ceiling-C [ppm]	Ceiling-C [mg/m ³]	Notation	Source
AU	hexylene glycol (2-methylpentane-2,4-diol)	107-41-5	WES					25	121		WES

Notation

Ceiling-C Ceiling value is a limit value above which exposure should not occur

STEL Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)

TWA Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified)

Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	44.4 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	49 mg/m ³	human, inhalatory	worker (industry)	chronic - local effects
DNEL	98 mg/m ³	human, inhalatory	worker (industry)	acute - local effects
DNEL	42 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

2-Methyl-2,4-pentandiol $\geq 99\%$, for synthesis

article number: CN17

Environmental values

Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0.429 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0.043 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	20 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	1.59 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0.159 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0.066 mg/kg	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



• hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

• type of material

Butyl caoutchouc (butyl rubber)

• material thickness

0,4 mm

• breakthrough times of the glove material

>480 minutes (permeation: level 6)

• Splash protection - Protective gloves

• type of material: NBR (Nitrile rubber)

• material thickness: >0,11 mm

• breakthrough times of the glove material: >240 minutes (permeation: level 5)

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentanediol $\geq 99\%$, for synthesis

article number: CN17

• other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of $> 65\text{ }^{\circ}\text{C}$, colour code: Brown).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	colourless
Odour	mild sweet
Odour threshold	50 ppm
Melting point/freezing point	$-40\text{ }^{\circ}\text{C}$ at 1,013 hPa
Boiling point or initial boiling point and boiling range	$196\text{ }^{\circ}\text{C}$ at 1,013 hPa
Flammability	flammable liquid in accordance with GHS criteria
Lower and upper explosion limit	1.3 vol% (LEL) - 7.4 vol% (UEL)
Flash point	$93\text{ }^{\circ}\text{C}$ (c.c.)
Auto-ignition temperature	$306\text{ }^{\circ}\text{C}$
Decomposition temperature	not relevant
pH (value)	not determined (neutral)
Kinematic viscosity	$36.96\text{ mm}^2/\text{s}$ at $20\text{ }^{\circ}\text{C}$
Dynamic viscosity	34 mPa s at $20\text{ }^{\circ}\text{C}$
<u>Solubility(ies)</u>	
Water solubility	miscible in any proportion
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	0.5802 (ECHA)
Soil organic carbon/water (log KOC)	0 (ECHA)
Vapour pressure	0.07 hPa at $20\text{ }^{\circ}\text{C}$

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentanediol ≥99 %, for synthesis

article number: **CN17**

Density and/or relative density

Density 0.92 g/cm³ at 20 °C

Relative vapour density 4.07 (air = 1)

Particle characteristics not relevant (liquid)

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard classes: There is no additional information.

Other safety characteristics:

Miscibility completely miscible with water

Refractive index 1.424 – 1.43

SECTION 10: Stability and reactivity

10.1 Reactivity

It's a reactive substance. Risk of ignition.

If heated

Risk of ignition. Vapours may form explosive mixtures with air.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser, Mineral acids

10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

10.5 Incompatible materials

Rubber articles, different plastics

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Shall not be classified as acutely toxic.

GHS of the United Nations, annex 4. May be harmful if swallowed.

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentanediol $\geq 99\%$, for synthesis

article number: CN17

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	3,700 mg/kg	rat		TOXNET
dermal	LD50	7,900 mg/kg	rabbit		TOXNET

Skin corrosion/irritation

Causes skin irritation.

Serious eye damage/eye irritation

Causes serious eye irritation.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Suspected of damaging the unborn child.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

vomiting, nausea

• If in eyes

Causes serious eye irritation

• If inhaled

Data are not available.

• If on skin

causes skin irritation

• Other information

Other adverse effects: Headache, Vertigo, Spasms, Dyspnoea, Unconsciousness

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentanediol $\geq 99\%$, for synthesis

article number: CN17

SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	9,910 mg/l	fish	ECHA	96 h
EC50	5,410 mg/l	aquatic invertebrates	ECHA	48 h
ErC50	>429 mg/l	algae	ECHA	72 h

12.2 Persistence and degradability

Theoretical Oxygen Demand: 2.302 mg/mg
Theoretical Carbon Dioxide: 2.235 mg/mg

Biodegradation

The substance is readily biodegradable.

Process of degradability		
Process	Degradation rate	Time
biotic/abiotic	70 %	10 d
oxygen depletion	81 %	28 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	0.5802 (ECHA)
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12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	0 (ECHA)
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12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

12.7 Other adverse effects

Data are not available.

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentanediol $\geq 99\%$, for synthesis

article number: CN17

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

SECTION 14: Transport information

- | | | |
|------|---|---|
| 14.1 | UN number | not subject to transport regulations |
| 14.2 | UN proper shipping name | not assigned |
| 14.3 | Transport hazard class(es) | not assigned |
| 14.4 | Packing group | not assigned |
| 14.5 | Environmental hazards | non-environmentally hazardous acc. to the dangerous goods regulations |
| 14.6 | Special precautions for user | There is no additional information. |
| 14.7 | Transport in bulk according to IMO instruments | The cargo is not intended to be carried in bulk. |
| 14.8 | <u>Information for each of the UN Model Regulations</u> | |
| | Transport information National regulations Additional information (UN RTDG) | Not subject to transport regulations. UN RTDG |
| | International Maritime Dangerous Goods Code (IMDG) - Additional information | Not subject to IMDG. |
| | International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information | Not subject to ICAO-IATA. |

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentanediol ≥99 %, for synthesis

article number: CN17

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

There is no additional information.

National regulations(Australia)

Australian Inventory of Chemical Substances(AICS)

Substance is listed.

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

Legend

AIIC	Australian Inventory of Industrial Chemicals
CICR	Chemical Inventory and Control Regulation
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

2-Methyl-2,4-pentanediol $\geq 99\%$, for synthesis

article number: CN17

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.1		Classification acc. to GHS: change in the listing (table)	yes
2.2		Pictograms: change in the listing (table)	yes
2.2		Hazard statements: change in the listing (table)	yes
2.2		Precautionary statements - response: change in the listing (table)	yes
2.2		Precautionary statements - disposal: change in the listing (table)	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	Ceiling value
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
ErC50	\equiv EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
LEL	Lower explosion limit (LEL)
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



2-Methyl-2,4-pentanediol $\geq 99\%$, for synthesis

article number: **CN17**

Abbr.	Descriptions of used abbreviations
ppm	Parts per million
STEL	Short-term exposure limit
TWA	Time-weighted average
UEL	Upper explosion limit (UEL)
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative
WES	Safe Work Australia: Workplace exposure standards for airborne contaminants

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H227	Combustible liquid.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H361d	Suspected of damaging the unborn child.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.